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=> fil casreact
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FILE CONTENT:1840 - 9 Jul 2006 VOL 145 ISS 2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*                                                            *
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provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d sta que l2
L1              STR

RRT
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NODE ATTRIBUTES:
CONNECT IS E2  RC AT   7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
L2          140 SEA FILE=CASREACT SSS FUL L1 (  1518 REACTIONS)

100.0% DONE 1090410 VERIFIED    1518 HIT RXNS (     4 INCOMP)     140 DOCS
SEARCH TIME: 00.00.20

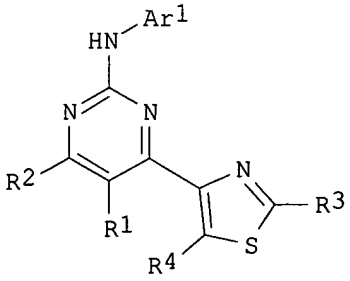

=> d bib abs fhit retable tot


L48  ANSWER 1 OF 2  CASREACT  COPYRIGHT 2006 ACS on STN
AN   141:332212  CASREACT
TI   Preparation of aminopyrimidinyl-substituted thiazoles useful as inhibitors
```

of protein kinases
IN Farmer, Luc J.; Harrington, Edmund Martin; Salituro, Francesco G.; Wang, Jian
PA **Vertex Pharmaceuticals Incorporated, USA**
SO PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004087698	A2	20041014	WO 2004-US9061	20040325
	WO 2004087698	A3	20041209		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004225965	A1	20041014	AU 2004-225965	20040325
	CA 2523125	AA	20041014	CA 2004-2523125	20040325
	US 2004235834	A1	20041125	US 2004-809944	20040325
	EP 1610793	A2	20060104	EP 2004-758287	20040325
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				

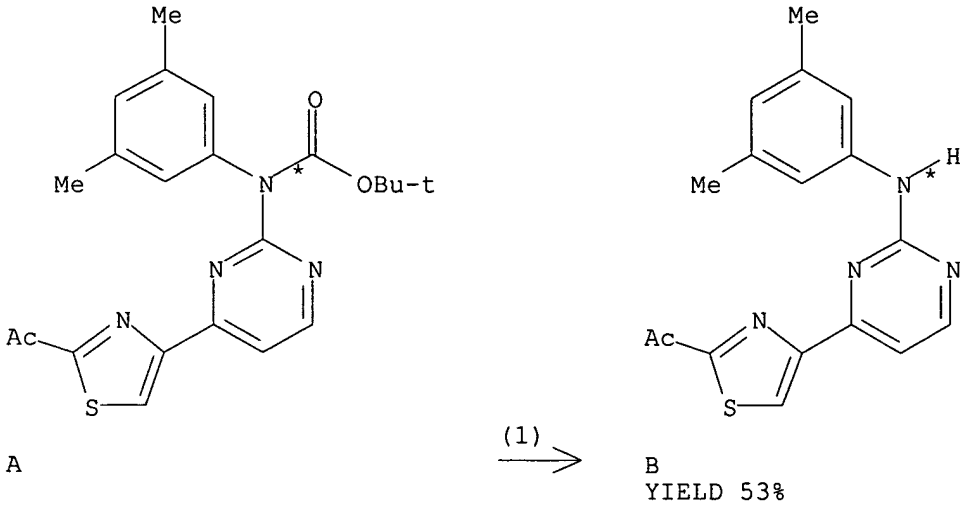
PRAI US 2003-457218P 20030325
WO 2004-US9061 20040325
OS MARPAT 141:332212
GI



I

AB Title compds. I [R1-2 = halo, CN, NO2, etc.; Ar1 = aryl, etc.; R3-4 = ZR7; Z = bond, alkylidene; R7 = halo, NO2, CN, alkoxy, etc.] are prepared General procedures are provided, e.g., [4-[2-((3,5-dimethylphenyl)amino)pyrimidin-4-yl]thiazol-2-yl]methanol. Selected example compds. of the invention exhibit Ki < 5 μM for Syk kinase. I are useful for the treatment of autoimmune disorders.

RX(1) OF 113 ...**A** ===> **B**

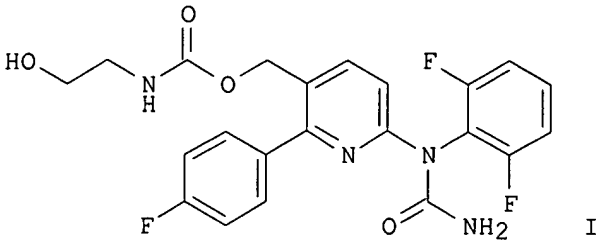


RX(1) RCT A **883967-53-1**
RGT C 76-05-1 F3CCO2H
PRO B **769933-80-4**
SOL 75-09-2 CH2Cl2
CON 1 hour, room temperature
NTE analogs similarly prepared

L48 ANSWER 2 OF 2 CASREACT COPYRIGHT 2006 ACS on STN
AN 141:225319 CASREACT
TI Process for preparation of N-heteroaryl-N-aryl-amines
IN **Snoonian, John R.; Oliver-Shaffer, Patrica-Ann**
PA **Vertex Pharmaceuticals Incorporated, USA**
SO PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004072038	A1	20040826	WO 2004-US3933	20040210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004212494	A1	20040826	AU 2004-212494	20040210
CA 2515669	AA	20040826	CA 2004-2515669	20040210
US 2004230058	A1	20041118	US 2004-775687	20040210
EP 1603878	A1	20051214	EP 2004-709916	20040210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1761653	A	20060419	CN 2004-80007137	20040210
NO 2005004201	A	20051006	NO 2005-4201	20050909

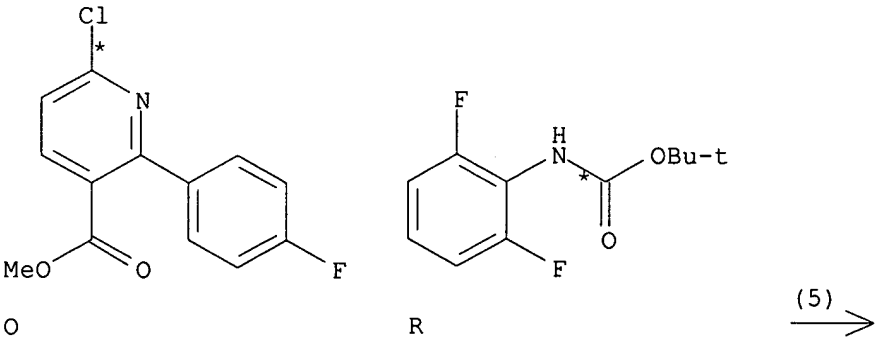
PRAI US 2003-446641P 20030210
US 2003-474272P 20030528
WO 2004-US3933 20040210
OS MARPAT 141:225319
GI



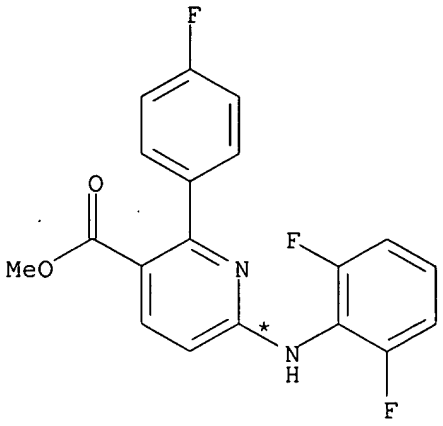
I

AB The present invention relates to a process for producing diarylamine derivs. with general formula of Ar1-NH-Ar2 [wherein Ar1 and Ar2 = independently (un)substituted aryl or heteroaryl] or salts thereof, which comprises coupling a compound of formula Ar1-X [where X = a leaving group] with an amine of formula Ar2-NH-Y [where Y = CO2Z; Z = alkyl, PhCH2, Fmoc, etc.] in the presence of an alkali metal salt or a transition metal catalyst. For example, the compound I was prepared starting from 6-chloro-2-(4-fluorophenyl)nicotinic acid Me ester (preparation given) and N-(tert-butoxycarbonyl)-2,6-difluoroaniline.

RX(5) OF 37 ...O + **R** ===> **S**...



O R (5)



S

RX(5)

STAGE(1)
RGT T 98327-87-8 Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl-
CAT 3375-31-3 Pd(OAc)2
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 2 hours, room temperature -> 50 deg C
SUBSTAGE(2) 50 deg C -> 30 deg C

STAGE(2)
RCT O 745833-06-1, R **745833-17-4**
RGT U 7778-53-2 K3PO4
CON SUBSTAGE(2) overnight, 100 deg C

STAGE(3)
RGT V 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(2) overnight

PRO S **745833-08-3**
NTE workup

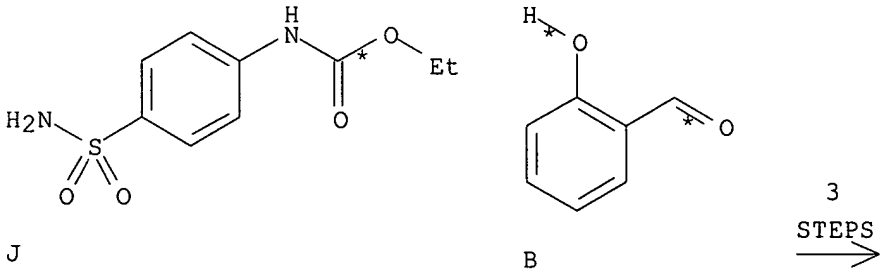
=> d bib abs fhit retable tot 147

L47 ANSWER 1 OF 3 CASREACT COPYRIGHT 2006 ACS on STN
AN 139:331783 CASREACT
TI Synthesis, spectral and magnetic studies of mononuclear and binuclear Mn(II), Co(II), Ni(II) and Cu(II) complexes with semicarbazone ligands derived from sulfonamide
AU Saleh, A. A.; Khalil, S. M. E.; Eid, M. F.; El-Ghamry, M. A.
CS Department of Chemistry, Faculty of Education, Ain Shams University, Cairo, Egypt
SO Journal of Coordination Chemistry (**2003**), 56(6), 467-480
CODEN: JCCMBQ; ISSN: 0095-8972
PB Taylor & Francis Ltd.
DT Journal

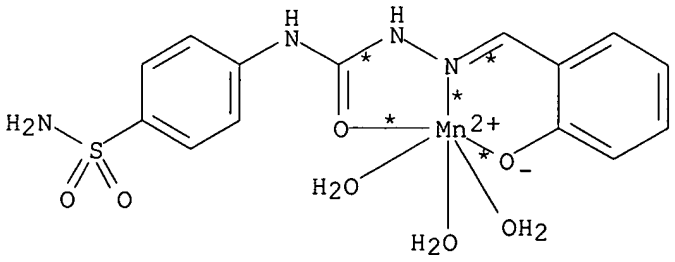
LA English

AB Mononuclear and binuclear Mn(II), Co(II), Ni(II) and Cu(II) complexes of new semicarbazone ligands derived from sulfonamide were synthesized and characterized by elemental anal. and IR spectra. In mononuclear complexes, the semicarbazone behaves as a monoanionic terdentate or neutral terdentate ligand towards the metal ion. However, in binuclear complexes, it behaves as a monoanionic terdentate towards one of the bivalent metal ions and monoanionic bidentate ligand towards the other metal ion in the same complex. Electronic spectra and magnetic susceptibility measurements of the solid complexes indicated octahedral geometry around Mn(II), Co(II) and Ni(II) and square planar around the Cu(II) ion. These geometries were confirmed by the results obtained from thermal analyses. The antifungal properties of the ligands and their complexes were studied.

RX(44) OF 79 COMPOSED OF RX(5), RX(1), RX(7)
RX(44) **J** + B ===> **N**



J B



● Cl^-

● 3 H_2O

N

RX(5) RCT J **41104-55-6**
RGT K 7803-57-8 N2H4-H2O
PRO A 87013-80-7

SOL 68-12-2 DMF
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, reflux

RX(1) RCT A 87013-80-7, B 90-02-8
PRO C 613221-31-1
SOL 68-12-2 DMF
CON 1 hour, reflux
NTE product depends on time of refluxing

RX(7) RCT C 613221-31-1

STAGE(1)
RGT O 1310-65-2 LiOH
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 30 minutes, room temperature

STAGE(2)
RGT P 7773-01-5 MnCl2
SOL 7732-18-5 Water
CON 5 hours, room temperature

PRO N **613221-35-5**

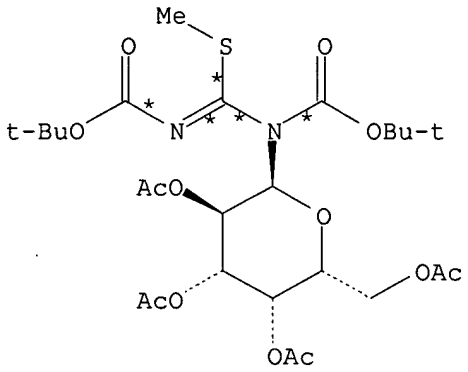
RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Biradar, N	1971	33	2451	J Inorg Nucl Chem	CAPLUS
Cotton, F	1961	83	4175	J Am Chem Soc	
Dhakarey, R	1985	32	35	J Chin Chem Soc	CAPLUS
Eugenio, J	1999	18	2483	Polyhedron	CAPLUS
Hathaway, B	1970	5	143	Coord Chem Rev	CAPLUS
Hueso, F	1999	18	351	polyhedron	
Ismail, T	2000	43	227	Egypt J Chem	CAPLUS
Khalil, S	2000	52	73	J Coord Chem	CAPLUS
Kulkarni, Y	1990	67	46	J Indian Chem Soc	CAPLUS
Lever, A	1968			Inorganic Electronic	
Nakamoto, K	1980		258	Infrared and Raman S	
Probhakaran, C	1998	75	7	J Indian Chem Soc	
Saleh, A	1990	29	2132	J Inorg Chem	CAPLUS
Satapathy, S	1970	32	2223	J Inorg Nucl Chem	CAPLUS
Satpathy, K	1986	68	377	J Indian Chem Soc	
Saxena, A	1981	43	3091	J Inorg Nucl Chem	CAPLUS
Singh, A	1996	73	339	J Indian Chem Soc	
Sonar, G	1995	72	677	J Indian Chem Soc	
West, D	1993	49	123	Coord Chem Rev	

L47 ANSWER 2 OF 3 CASREACT COPYRIGHT 2006 ACS on STN
AN 139:7095 CASREACT
TI Syntheses of guanidinoglycosides with the inventive use of Mitsunobu conditions and 1,8-diazabicyclo[5.4.0]undec-7-ene
AU Lin, Peishan; Heng, Sabrina Cher Hui; Sim, Mui Mui
CS Institute of Molecular and Cell Biology, Singapore, 117609, Singapore
SO Synthesis (**2003**), (2), 255-261
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
AB A series of novel guanidinoglycosides was successfully synthesized. This

was accomplished with the use of Mitsunobu conditions as a strategy to convert the glycopyranose anomeric hydroxy group to give the corresponding substituted masked guanidines in high yields. Subsequent deprotection and coupling with Fmoc protected β-amino acid, afforded a series of N,N'-substituted-methylisothioureas. Cleavage of Fmoc followed by concomitant cyclization was achieved with a catalytic amount of DBU to give the guanidinoglycosides.

RX(32) OF 41 COMPOSED OF RX(3), RX(11), RX(6)
RX(32) **I** + T ===> **AA**



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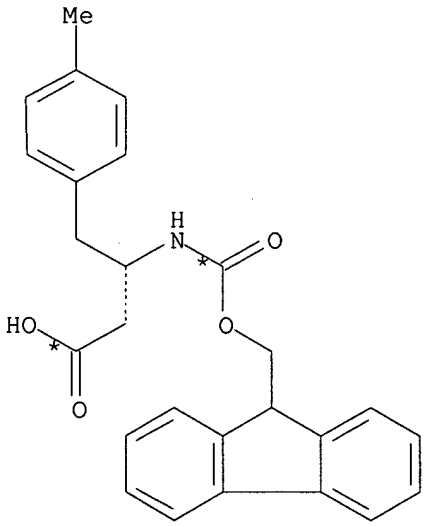

T

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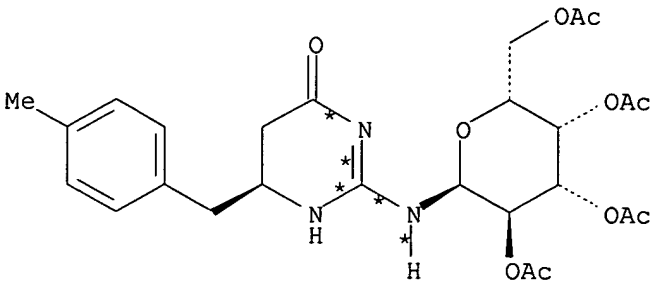
STEPS



AA
YIELD 45%

RX(3) RCT I **535952-55-7**

STAGE(1)
RGT L 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2, 100-66-3 PhOMe
CON 15 minutes, 0 deg C

STAGE(2)
SOL 110-54-3 Hexane

STAGE(3)
SOL 67-56-1 MeOH

STAGE(4)
RGT M 144-55-8 NaHCO3
CON neutralized

PRO K 535952-59-1

RX(11) RCT T 270062-97-0

STAGE(1)
RGT V 2592-95-2 1-Benzotriazolol, W 693-13-0 i-PrN:C:NPr-i
SOL 127-19-5 AcNMe2, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

STAGE(2)
RCT K 535952-59-1
RGT X 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2
CON 24 hours, room temperature

PRO Z 535952-62-6
NTE stereoselective

RX(6) RCT Z 535952-62-6
RGT AB 6674-22-2 DBU
PRO AA **535952-67-1**
SOL 109-99-9 THF
CON 1 hour, room temperature
NTE stereoselective

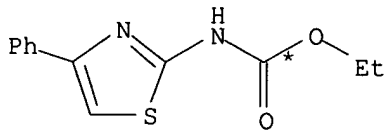
RETABLE

Referenced Author	Year	VOL	PG	Referenced Work	Referenced

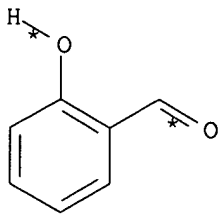
(RAU)	(RPY)	(RVL)	(RPG)	(RWK)	File
Baker, T	2000	65	9054	J Org Chem	CAPLUS
Bu, X	2002	43	2419	Tetrahedron Lett	CAPLUS
Cotner, E	1998	63	1737	J Org Chem	CAPLUS
Delaware, D	1986	39	251	J Antibiot	CAPLUS
Dodd, D	1994	35	977	Tetrahedron Lett	CAPLUS
Dodd, D	1998	39	5701	Tetrahedron Lett	CAPLUS
Feichtinger, K	1998	63	3804	J Org Chem	CAPLUS
Feichtinger, K	1998	63	8432	J Org Chem	CAPLUS
Gololobov, Y	1981	37	437	Tetrahedron	CAPLUS
Hughes, D	1996	28	127	Org Prep Proced Int	CAPLUS
Kim, H	1999	2	193	Synlett	
Lemieux, R	1948	3	337	Adv Carbohydr Chem	CAPLUS
Lin, P	2001	66	8243	J Org Chem	CAPLUS
Magri, N	1988	51	298	J Nat Prod	CAPLUS
Maurin, M	2001	45	2977	Antimicrob Agents Ch	CAPLUS
Metcalf, C	1998	39	3435	Tetrahedron Lett	CAPLUS
Mitsunobu, O	1981		1	Synthesis	CAPLUS
Molina, P	1994		1197	Synthesis	CAPLUS
Mori, Y	1999	40	7239	Tetrahedron Lett	CAPLUS
Ouyang, X	1999	55	8295	Tetrahedron	CAPLUS
Reitz, A	1989	32	2110	J Med Chem	CAPLUS
Roush, W	1994	28	4935	Tetrahedron Lett	
Sheppeck, J	2000	41	5329	Tetrahedron Lett	CAPLUS
Wade, J	1991	4	194	Pept Res	CAPLUS

L47 ANSWER 3 OF 3 CASREACT COPYRIGHT 2006 ACS on STN
AN 138:361747 CASREACT
TI Synthesis and antimicrobial activity of copper-, cobalt- and nickel(II) complexes with Schiff bases
AU Jadegoud, Y.; Ijare, Omkar B.; Mallikarjuna, N. N.; Angadi, S. D.; Mruthyunjayaswamy, B. H. M.
CS Department of Chemistry, Gulbarga University, Gulbarga, 585 106, India
SO Journal of the Indian Chemical Society (**2002**), 79(12), 921-924
CODEN: JICSAH; ISSN: 0019-4522
PB Indian Chemical Society
DT Journal
LA English
AB A few complexes of CuII, CoII and NiII were prepared by reacting their metal(II) chlorides with 3-(4'-phenylthiazole-2'-yl)-1-(2'-hydroxy-1'-iminomethylphenyl)urea and with 3-(4'-phenylthiazole-2'-yl)-1-(2',4'-dihydroxy/2'-hydroxy-5'-chloro-1'-methyliminomethylphenyl)ureas (Schiff bases) in EtOH medium. The chelates are colored solids and nonelectrolytes ML2. The IR spectra of the ligands and complexes suggest involvement of o-hydroxy group, carbonyl group, azomethine group in bonding through O and N atoms resp. The electronic spectra and magnetic data suggest the octahedral stereochem. for all the complexes in which metal(II) ion exhibits coordination number six. The ligands and complexes were tested for their antimicrobial activity.

RX(31) OF 48 COMPOSED OF RX(14), RX(10), RX(1)
RX(31) 2 **Y** + 2 R ===> **B**



2 Y



2 R

3
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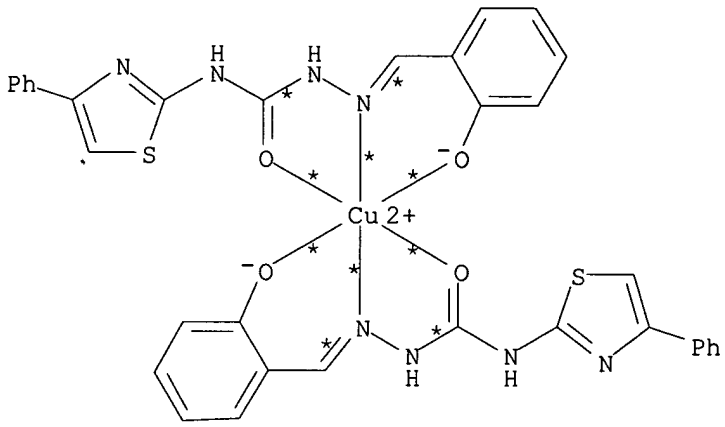

B
YIELD 88%

RX(14) RCT Y **3673-36-7**
RGT AA 302-01-2 N2H4
PRO S 519141-81-2
SOL 64-17-5 EtOH
CON 5 hours, reflux

RX(10) RCT R 90-02-8, S 519141-81-2
PRO A 519141-78-7
CAT 7647-01-0 HCl
SOL 64-17-5 EtOH
CON 8 hours, reflux

RX(1) RCT A 519141-78-7

STAGE(1)
RGT C 7447-39-4 CuCl2
SOL 64-17-5 EtOH
CON 2 hours, reflux

STAGE(2)
RGT D 127-09-3 AcONa
CON 3 hours, reflux

PRO B **519141-69-6**

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Biradar, N	1971	33	2451	J Inorg Nucl Chem	CAPLUS
Chohan, Z	1998	28	1673	Synth React Inorg Me	CAPLUS
Deshpande, V	1986		2397	Angew Makromol Sci C	
Dey, K	1999	38	1139	Indian J Chem, Sect	
Dilworh, I	1976	21	29	Coord Chem Rev	
Dodson, R	1945	67	2242	J Am Chem Soc	CAPLUS
Dunn, T	1960			The Visible and Ultr	
Durig, J	1967	23	1121	Spectrochim Acta	CAPLUS
Dutta, R	1985	44	635	J Sci Ind Res	CAPLUS
Feggis, B	1966			Introduction to Liga	
Freedman, H	1961	83	2900	J Am Chem Soc	CAPLUS
Hiremath, A	1982	59	1017	J Indian Chem Soc	
Hiremath, A	1984	61	191	J Indian Chem Soc	CAPLUS
Holm, R	1966	7	83	Prog Inorg Chem	CAPLUS
Ibrahim, K	1993	32	361	Indian J Chem, Sect	
Kato, M	1964	64	99	Chem Rev	CAPLUS
Krishna, C	1977	39	1253	J Inorg Nucl Chem	
Mane, R	1983	22	81	Indian J Chem, Sect	
Pelizzi, C	1980		1970	J Chem Soc, Dalton T	CAPLUS
Prabhakaran, C	1980	20	474	Indian J Chem Sect A	
Rajashekar, G	1998	10	306	Asian J Chem	
Rastogi, D	1979	8	97	J Coord Chem	
Tahir, A	2000	39	450	Indian J Chem, Sect	
Thaker, B	1996	35	483	Indian J Chem, Sect	
Tijmir, H	1983	2	723	Polyhedron	

=> => fil reg
FILE 'REGISTRY' ENTERED AT 09:05:24 ON 12 JUL 2006

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUL 2006 HIGHEST RN 892124-43-5
DICTIONARY FILE UPDATES: 11 JUL 2006 HIGHEST RN 892124-43-5

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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d que 169
L49 69304 SEA FILE=HCAPLUS ABB=ON PLU=ON ALKALI METAL?/CT
L50 583318 SEA FILE=HCAPLUS ABB=ON PLU=ON "ALKALI METAL SALTS"+OLD,NT/CT

```
L51       635713 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L49 OR L50)
L52        89263 SEA FILE=HCAPLUS ABB=ON  PLU=ON  TRANSITION METAL?/CT
L53         8286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("TRANSITION METALS, USES"/CT
                 OR "TRANSITION METALS, USES AND MISCELLANEOUS"/CT)
L54       669385 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L51 OR L52 OR L53) AND
                 (PY<=2003 OR PRY<=2003 OR AY<=2003)
L55        14006 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L54 AND HET?/SC,SX
L56          155 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND ("COUPLING AGENTS"+OLD
                 ,NT/CT OR "COUPLING FACTORS"/CT OR "COUPLING REACTION"+OLD,NT/C
                 T)
L57           76 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND "COUPLING REACTION
                 CATALYSTS"+OLD,NT/CT
L58            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND ("COUPLING REACTION
                 ENTHALPY"+OLD,NT/CT OR "COUPLING REACTION KINETICS"+OLD,NT/CT
                 OR "COUPLING REACTIONS"/CT)
L59          175 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L56 OR L57 OR L58)
L60          120 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L59 AND HET?/SC
L62              TRANSFER  PLU=ON  L60 1- RN :    4093 TERMS
L63         4093 SEA FILE=REGISTRY ABB=ON  PLU=ON  L62
L64              STR

Cy~^N~^Hy
 1   2   3


NODE ATTRIBUTES:
CONNECT IS E2  RC AT   2
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L69          616 SEA FILE=REGISTRY SUB=L63 SSS FUL L64


=> d que l74
L49        69304 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ALKALI METAL?/CT
L50       583318 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "ALKALI METAL SALTS"+OLD,NT/CT

L51       635713 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L49 OR L50)
L52        89263 SEA FILE=HCAPLUS ABB=ON  PLU=ON  TRANSITION METAL?/CT
L53         8286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("TRANSITION METALS, USES"/CT
                 OR "TRANSITION METALS, USES AND MISCELLANEOUS"/CT)
L54       669385 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L51 OR L52 OR L53) AND
                 (PY<=2003 OR PRY<=2003 OR AY<=2003)
L55        14006 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L54 AND HET?/SC,SX
L56          155 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND ("COUPLING AGENTS"+OLD
                 ,NT/CT OR "COUPLING FACTORS"/CT OR "COUPLING REACTION"+OLD,NT/C
                 T)
L57           76 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND "COUPLING REACTION
                 CATALYSTS"+OLD,NT/CT
L58            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L55 AND ("COUPLING REACTION
                 ENTHALPY"+OLD,NT/CT OR "COUPLING REACTION KINETICS"+OLD,NT/CT
                 OR "COUPLING REACTIONS"/CT)
L59          175 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L56 OR L57 OR L58)
L60          120 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L59 AND HET?/SC
L62              TRANSFER  PLU=ON  L60 1- RN :    4093 TERMS
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L63         4093 SEA FILE=REGISTRY ABB=ON  PLU=ON  L62
L66              STR
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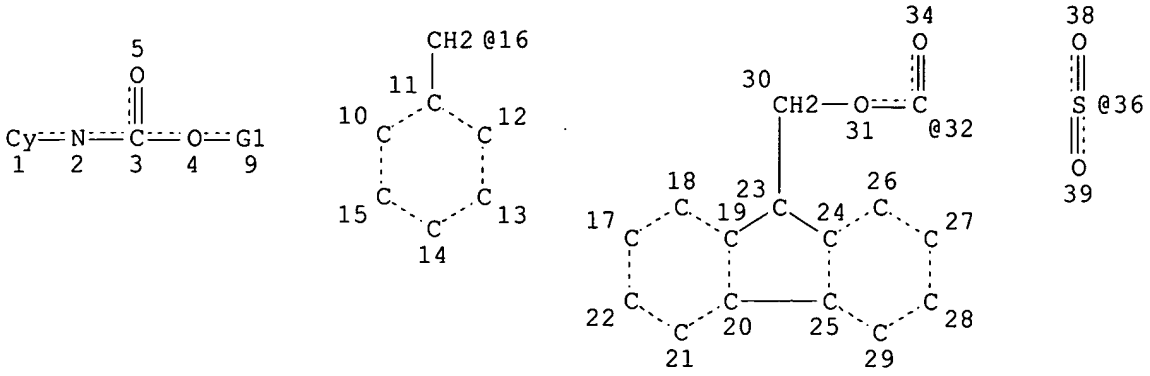


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VAR G1=AK/16/32/36/CY
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  33

STEREO ATTRIBUTES: NONE
L74           30 SEA FILE=REGISTRY SUB=L63 SSS FUL L66


=> d his

     (FILE 'HOME' ENTERED AT 08:25:28 ON 12 JUL 2006)
               SET COST OFF

     FILE 'CASREACT' ENTERED AT 08:25:48 ON 12 JUL 2006
               ACT ZINNA775B/A
              ---------
L1             STR
L2           140 SEA FILE=CASREACT SSS FUL L1 (  1518 REACTIONS)
              ---------
               ACT ZINNA775A/Q
              ---------
L3             STR
              ---------
L4             STR L3
L5             3 S L4 SAM SUB=L2
L6           139 S L4 FUL SUB=L2
               SAV L6 ZINNA775E/A
L7             1 S L2 AND (SNOONIAN? OR OLIVER? OR SHAFFER?)/AU
L8             1 S L6 AND (SNOONIAN? OR OLIVER? OR SHAFFER?)/AU
L9             2 S L2,L6 AND VERTEX?/PA,CS
L10            2 S L7-L9
L11          106 S L2 AND (PY<=2003 OR PRY<=2003 OR AY<=2003)
               ACT ZINNA775C/A
              ---------
L12 (       4892)SEA FILE=CASREACT ABB=ON  PLU=ON  ("TRANSITION METAL ALLOYS"/CT
L13 (      17604)SEA FILE=CASREACT ABB=ON  PLU=ON  (ALKALI OR TRANSITION)(L)META
L14        17604 SEA FILE=CASREACT ABB=ON  PLU=ON  (L12 OR L13)
              ---------
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```
L15         2358 S ALKALI METAL?/CT
L16         4892 S TRANSITION METAL?/CT
L17            3 S L11 AND L15,L16
L18            2 S L17 NOT L10
                 E COUPLING/CT
L19            2 S E4-E8 AND L11
L20            1 S L10 AND L17,L19
L21            2 S L10,L20
L22            3 S L17-L20 NOT L21
L23          101 S L11 NOT L21,L22

     FILE 'HCAPLUS' ENTERED AT 08:35:42 ON 12 JUL 2006
                 ACT ZINNA775D/A
                 ---------
L24 (          1)SEA FILE=HCAPLUS ABB=ON  PLU=ON  US20040230058/PN OR US2004-775
L25 (         16)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("SNOONIAN J R"/AU OR "SNOONIA
L26 (          4)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("OLIVER SHAFFER PATRICA ANN"/
L27 (         23)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("OLIVER P"/AU OR "OLIVER P A"
L28 (         13)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("OLIVER PATRICIA"/AU OR "OLIV
L29 (         24)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("SHAFFER P"/AU OR "SHAFFER P
L30 (          2)SEA FILE=HCAPLUS ABB=ON  PLU=ON  "SHAFFER PATRICIA"/AU
L31 (        683)SEA FILE=HCAPLUS ABB=ON  PLU=ON  VERTEX?/PA,CS
L32          759 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L24 OR L25 OR L26 OR L27 OR L
                 ---------
L33            1 S L24 AND US20040230058/PN
                 SEL RN

     FILE 'REGISTRY' ENTERED AT 08:36:31 ON 12 JUL 2006
L34           29 S E1-E29
L35           16 S L34 NOT NC5/ES
L36           14 S L35 NOT C6/ES

     FILE 'HCAPLUS' ENTERED AT 08:38:28 ON 12 JUL 2006

     FILE 'CASREACT' ENTERED AT 08:38:42 ON 12 JUL 2006
L37       159260 S L36
L38            2 S L37 AND L21
L39            1 S L37 AND L22
L40            2 S L22 NOT L39
L41           75 S L23 AND L37

     FILE 'REGISTRY' ENTERED AT 08:41:20 ON 12 JUL 2006
L42           11 S L36 AND (PD OR RB OR CS OR K OR NA)/ELS
L43            3 S L36 NOT L42
L44            1 S L43 AND H5NO

     FILE 'HCAPLUS' ENTERED AT 08:42:11 ON 12 JUL 2006

     FILE 'CASREACT' ENTERED AT 08:42:24 ON 12 JUL 2006
L45           60 S L42,L44 AND L23
L46            5 S L21,L22 AND (PY<=2003 OR PRY<=2003 OR AY<=2003)
L47            3 S L46 NOT L21

     FILE 'CASREACT' ENTERED AT 08:44:03 ON 12 JUL 2006
L48            2 S L46 NOT L47

     FILE 'HCAPLUS' ENTERED AT 08:47:03 ON 12 JUL 2006
                 E ALKALI METAL/CT
                 E ALKALI METAL?/CT
L49        69304 S ALKALI METAL?/CT
```

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                E ALKALI METAL/CT
                E ALKALI METAL SALT/CT
L50        583318 S E4+OLD,NT
L51        635713 S L49,L50
                E TRANSITION METAL/CT
L52         89263 S TRANSITION METAL?/CT
                E TRANSITION METALS, /CT
L53          8286 S E18,E19
L54        669385 S L51-L53 AND (PY<=2003 OR PRY<=2003 OR AY<=2003)
L55         14006 S L54 AND HET?/SC,SX
                E COUPLING/CT
L56           155 S L55 AND (E6+OLD,NT OR E14 OR E21+OLD,NT)
L57            76 S L55 AND E58+OLD,NT
L58             3 S L55 AND (E66+OLD,NT OR E67+OLD,NT OR E72)
L59           175 S L56-L58
L60           120 S L59 AND HET?/SC
L61            55 S L59 NOT L60

     FILE 'REGISTRY' ENTERED AT 08:56:48 ON 12 JUL 2006

     FILE 'HCAPLUS' ENTERED AT 08:56:49 ON 12 JUL 2006
L62             TRA L60 1- RN :     4093 TERMS

     FILE 'REGISTRY' ENTERED AT 08:56:54 ON 12 JUL 2006
L63          4093 SEA L62
L64               STR
L65            34 S L64 SAM SUB=L63
L66               STR L4
L67             0 S L66 SAM SUB=L63
L68            50 S L66
L69           616 S L64 FUL SUB=L63
                  SAV L69 ZINNA775F/A

     FILE 'HCAPLUS' ENTERED AT 08:59:19 ON 12 JUL 2006
L70             9 S L69 (L) PREP+NT/RL
L71             5 S L70 AND L60
L72             3 S L70 AND L42,L44

     FILE 'REGISTRY' ENTERED AT 09:01:20 ON 12 JUL 2006
L73            50 S L66 SAM
L74            30 S L66 FUL SUB=L63
                  SAV L74 ZINNA775G/A

     FILE 'HCAPLUS' ENTERED AT 09:02:01 ON 12 JUL 2006
L75             2 S L74 AND L70
L76             3 S L72,L75
L77             2 S L71 NOT L76
L78             1 S L70 AND VERTEX?/PA,CS
L79             1 S L70 AND (SNOONIAN? OR OLIVER/ OR SHAFFER?)/AU
L80             1 S L78,L79
L81             5 S L76-L80
L82             5 S L81 AND L32,L33,L49-L61,L70-L72,L75-L81
L83             4 S L70 NOT L82

     FILE 'REGISTRY' ENTERED AT 09:05:24 ON 12 JUL 2006

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 09:05:40 ON 12 JUL 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 12 Jul 2006 VOL 145 ISS 3
FILE LAST UPDATED: 11 Jul 2006 (20060711/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l82 bib abs hitrn fhitstr retable

L82 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:1037107 HCAPLUS
DN 142:23304
TI Preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases
IN Traquandi, Gabriella; Brasca, Maria Gabriella; D'Alessio, Roberto; Polucci, Paolo; Roletto, Fulvia; Vulpetti, Anna; Pevarello, Paolo; Panzeri, Achille; Quartieri, Francesca; Ferguson, Ron; Vianello, Paola; Fancelli, Daniele
PA Pharmacia Italia S.A., Italy
SO PCT Int. Appl., 226 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004104007	A1	20041202	WO 2004-EP50612	20040427 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004240772	A1	20041202	AU 2004-240772	20040427 <--
	CA 2526578	AA	20041202	CA 2004-2526578	20040427 <--
	EP 1636236	A1	20060322	EP 2004-741483	20040427 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	NO 2005005496	A	20060214	NO 2005-5496	20051121 <--
PRAI	US 2003-472661P	P	20030522 <--		

WO 2004-EP50612 W 20040427
OS MARPAT 142:23304
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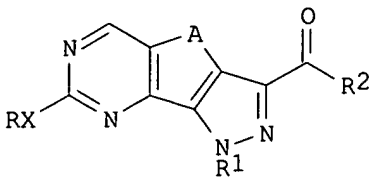
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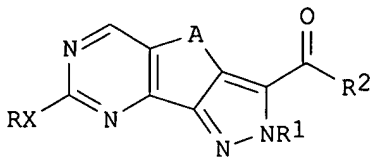
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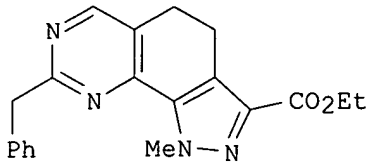
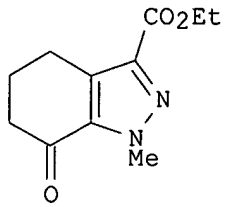

III


IV

AB Pyrazoloquinazolines I or II [A = CH2, CH2CH2, CH2CMe2, CMe2CH2, CH:CH; R = H, (un)substituted amino, alkyl, cycloalkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; R1 = H, (un)substituted alkyl, cycloalkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; R2 = (un)substituted amino, (hydroxy)amino; R1R2 = (CH2)2NH, (CH2)3NH; R3 = H, (un)substituted alkyl, cycloalkyl, aryl, aralkyl, heterocyclyl, heterocycloalkyl; RNR3 may also form a 5- or 6-membered heterocycle which may also contain a second heteroatom of N, O, or S; X = NR3, C(:O)NR3, NHC(:O)NH, O, S, SO2] such as pyrazolo[4,3-h]quinazoline III are prepared as inhibitors of protein kinases such as Aurora2 (and particularly cell cycle-dependent kinases) for the treatment of proliferative disorders such as cancer, Alzheimer's disease, viral infection, autoimmune diseases, and neurodegenerative disorders. Acid-catalyzed vinyl ether formation from 1,2-cyclohexanedione provides 2-ethoxy-2-cyclohexen-1-one; Claisen condensation with di-Et oxalate and cyclocondensation with Me hydrazine yields oxotetrahydroindazolecarboxylate IV. Dimethylaminomethylenation of IV with DMF di-tert-Bu acetal, cyclocondensation with methylisothiourea sulfate, and substitution of the methylthio group with benzylzinc bromide in the presence of tetrakis(triphenylphosphine)palladium yields III. I are active as protein kinase inhibitors and therefore as inhibitors of cellular proliferation (no data). Detailed processes for the preparation of compds. I (and intermediates prepared within) are claimed.

IT **802534-91-4P 802534-99-2P 802535-27-9P**
802535-57-5P 802535-81-5P 802535-83-7P
802537-13-9P 802537-15-1P 802537-24-2P
802537-25-3P 802537-26-4P 802537-27-5P
802537-28-6P 802537-29-7P 802537-30-0P
802537-31-1P 802537-32-2P 802537-33-3P
802537-34-4P 802537-35-5P 802537-36-6P
802537-37-7P 802537-38-8P 802537-39-9P
802537-92-4P 802537-93-5P 802537-94-6P
802537-96-8P 802537-98-0P 802538-79-0P
802539-63-5P 802539-65-7P 802539-70-4P
802539-81-7P
RL: PAC (Pharmacological activity); RCT (Reactant); **SPN (Synthetic**

preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases)

IT **802533-98-8P 802533-99-9P 802534-06-1P**
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RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**;
THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**
; USES (Uses)
(drug candidate; preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases)

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RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**;
THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**
; USES (Uses)
(drug candidate; preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases)

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RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(drug candidate; preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases)

IT **802541-68-0P 802541-69-1P 802541-70-4P**
802541-71-5P 802541-85-1P 802541-86-2P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases)

IT **7440-05-3**, Palladium, uses
RL: CAT (Catalyst use); USES (Uses)
(processes for the preparation of pyrazoloquinazoline protein kinase inhibitors)

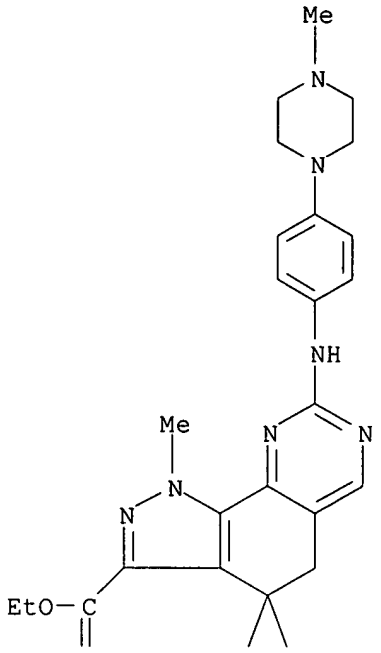
IT **534-17-8**, Cesium carbonate **1336-21-6**, Ammonium hydroxide **1907-33-1 4039-32-1**, Lithium bis(trimethylsilyl)amide
RL: RGT (Reagent); RACT (Reactant or reagent)
(processes for the preparation of pyrazoloquinazoline protein kinase inhibitors)

IT **802534-91-4P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; **PREP (Preparation)**; THU (Therapeutic use); **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrazoloquinazolines as inhibitors of protein kinases such as Aurora2 for the treatment of proliferative disorders such as cancer, Alzheimer's disease, and autoimmune diseases)

RN 802534-91-4 HCAPLUS
CN 1H-Pyrazolo[4,3-h]quinazoline-3-carboxylic acid, 4,5-dihydro-1,4,4-trimethyl-8-[[4-(4-methyl-1-piperazinyl)phenyl]amino]-, ethyl ester (9CI)

(CA INDEX NAME)

PAGE 1-A



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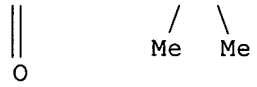

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Clare, M	2003			WO 03070706 A	HCAPLUS
Goldberg, D	2002			US 2002119975 A1	HCAPLUS
Masferrer, J	2004			WO 2004014352 A	HCAPLUS

=> d 182 bib abs hitstr retable 2-5

L82 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:696351 HCAPLUS
DN 141:225319
TI Process for preparation of N-heteroaryl-N-aryl-amines
IN **Snoonian, John R.; Oliver-Shaffer, Patrica-Ann**
PA **Vertex Pharmaceuticals Incorporated, USA**
SO PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DT Patent
LA English

FAN.CNT 1

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PI	WO 2004072038	A1	20040826	WO 2004-US3933	20040210 <--
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	CA 2515669	AA	20040826	CA 2004-2515669	20040210 <--
	US 2004230058	A1	20041118	US 2004-775687	20040210 <--
	EP 1603878	A1	20051214	EP 2004-709916	20040210 <--
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PRAI	US 2003-446641P	P	20030210 <--		
	US 2003-474272P	P	20030528 <--		
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OS CASREACT 141:225319; MARPAT 141:225319

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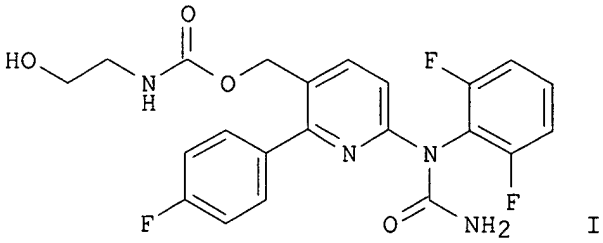


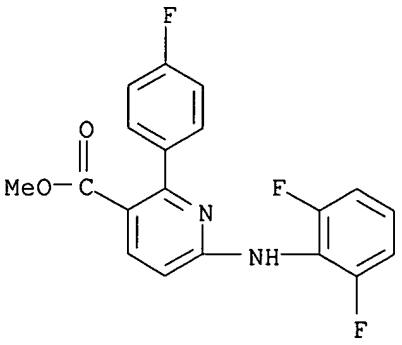
I

AB The present invention relates to a process for producing diarylamine derivs. with general formula of Ar1-NH-Ar2 [wherein Ar1 and Ar2 = independently (un)substituted aryl or heteroaryl] or salts thereof, which comprises coupling a compound of formula Ar1-X [where X = a leaving group] with an amine of formula Ar2-NH-Y [where Y = CO2Z; Z = alkyl, PhCH2, Fmoc, etc.] in the presence of an alkali metal salt or a transition metal catalyst. For example, the compound I was prepared starting from 6-chloro-2-(4-fluorophenyl)nicotinic acid Me ester (preparation given) and N-(tert-butoxycarbonyl)-2,6-difluoroaniline.

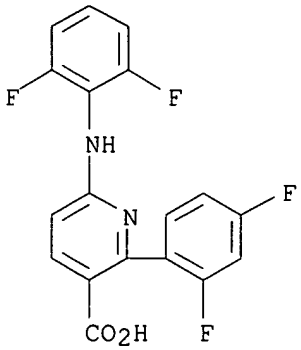
IT **745833-08-3P 745833-21-0P**
RL: **IMF (Industrial manufacture)**; RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of N-heteroaryl-N-aryl-amines)

RN 745833-08-3 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[(2,6-difluorophenyl)amino]-2-(4-fluorophenyl)-, methyl ester (9CI) (CA INDEX NAME)



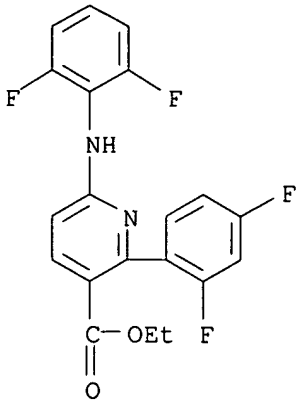
RN 745833-21-0 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2-(2,4-difluorophenyl)-6-[(2,6-difluorophenyl)amino]- (9CI) (CA INDEX NAME)



IT **7440-05-3**, Palladium, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of N-heteroaryl-N-aryl-amines)
RN 7440-05-3 HCAPLUS
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT **745833-15-2P**
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(preparation of N-heteroaryl-N-aryl-amines)
RN 745833-15-2 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2-(2,4-difluorophenyl)-6-[(2,6-difluorophenyl)amino]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

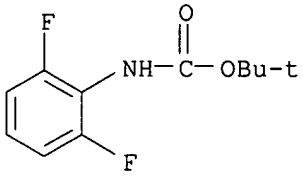


● HCl

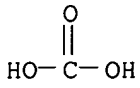
IT **1336-21-6**, Ammonium hydroxide **745833-17-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N-heteroaryl-N-aryl-amines)
RN 1336-21-6 HCAPLUS
CN Ammonium hydroxide ((NH4)(OH)) (9CI) (CA INDEX NAME)

H_4N-OH

RN 745833-17-4 HCAPLUS
CN Carbamic acid, (2,6-difluorophenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT **497-19-8**, Sodium carbonate, reactions **534-17-8**, Cesium carbonate **584-08-7**, Potassium carbonate **865-47-4** **865-48-5** **1310-73-2**, Sodium hydroxide, reactions **7440-09-7D**, Potassium, salts **7440-17-7D**, Rubidium, salts **7440-46-2D**, Cesium, salts **7778-53-2**, Potassium phosphate
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of N-heteroaryl-N-aryl-amines)
RN 497-19-8 HCAPLUS
CN Carbonic acid disodium salt (8CI, 9CI) (CA INDEX NAME)



●2 Na

RN 534-17-8 HCAPLUS
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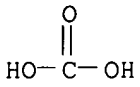

●2 Cs

RN 584-08-7 HCAPLUS
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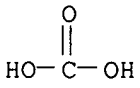

●2 K

RN 865-47-4 HCAPLUS
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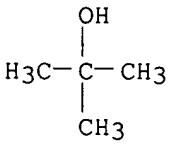
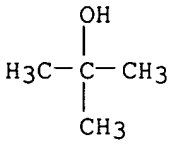


● K

RN 865-48-5 HCAPLUS
CN 2-Propanol, 2-methyl-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 1310-73-2 HCAPLUS
CN Sodium hydroxide (Na(OH)) (9CI) (CA INDEX NAME)

Na—OH

RN 7440-09-7 HCAPLUS
CN Potassium (8CI, 9CI) (CA INDEX NAME)

K

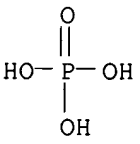
RN 7440-17-7 HCAPLUS
CN Rubidium (8CI, 9CI) (CA INDEX NAME)

Rb

RN 7440-46-2 HCAPLUS
CN Cesium (8CI, 9CI) (CA INDEX NAME)

Cs

RN 7778-53-2 HCAPLUS
CN Phosphoric acid, tripotassium salt (8CI, 9CI) (CA INDEX NAME)



●3 K

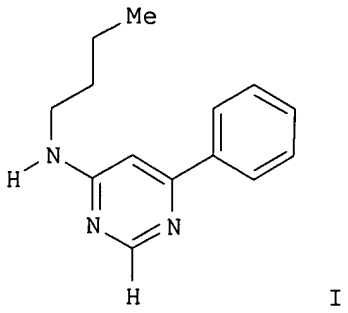
L82 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:98255 HCAPLUS
DN 138:287627
TI Suzuki Cross-Coupling of Solid-Supported Chloropyrimidines with

Arylboronic Acids

AU Wade, Janice V.; Krueger, Clinton A.
CS ChemRx Division, Discovery Partners International Inc., South San Francisco, CA, 94080, USA

SO Journal of Combinatorial Chemistry (**2003**), 5(3), 267-272
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
OS CASREACT 138:287627

GI

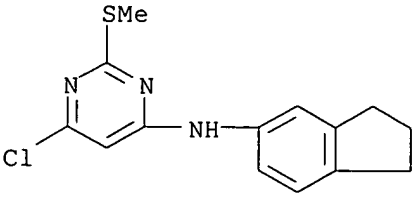


I

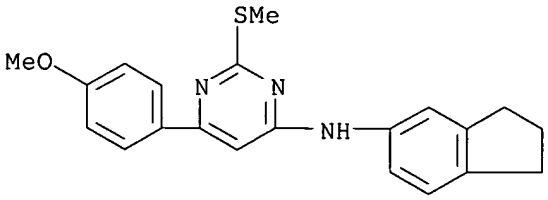
AB The utility of the Suzuki cross-coupling to synthesize biaryl compds. is expanded herein to include reactions of resin-supported chloropyrimidines with boronic acids. In particular, an efficient method is described for the synthesis of a library of biaryl compds. from solid-supported chloropyrimidines. The Suzuki reaction was performed in an inert atmospheric using Pd2(dba)3/P(t-Bu)3 as catalyst, spray-dried KF as base, and THF as solvent. The reaction was allowed to proceed overnight at 50 °C. Upon cleavage with acid, a library of 4-(substituted amino)-6-arylpyrimidines, e.g. I, was obtained in moderate yield and high purity.

IT **503610-74-0DP**, resin-supported **503610-79-5DP**, resin-supported
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(Suzuki cross-coupling of solid-supported chloropyrimidines with arylboronic acids)

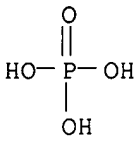
RN 503610-74-0 HCAPLUS
CN 4-Pyrimidinamine, 6-chloro-N-(2,3-dihydro-1H-inden-5-yl)-2-(methylthio)- (9CI) (CA INDEX NAME)



RN 503610-79-5 HCAPLUS
CN 4-Pyrimidinamine, N-(2,3-dihydro-1H-inden-5-yl)-6-(4-methoxyphenyl)-2-(methylthio)- (9CI) (CA INDEX NAME)

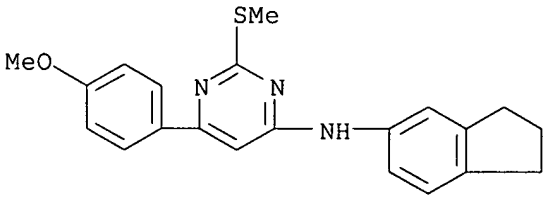


IT **7778-53-2**, Tripotassium phosphate
RL: RGT (Reagent); RACT (Reactant or reagent)
(Suzuki cross-coupling of solid-supported chloropyrimidines with arylboronic acids)
RN 7778-53-2 HCAPLUS
CN Phosphoric acid, tripotassium salt (8CI, 9CI) (CA INDEX NAME)

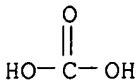


●3 K

IT **503610-79-5P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(Suzuki cross-coupling of solid-supported chloropyrimidines with arylboronic acids)
RN 503610-79-5 HCAPLUS
CN 4-Pyrimidinamine, N-(2,3-dihydro-1H-inden-5-yl)-6-(4-methoxyphenyl)-2-(methylthio)- (9CI) (CA INDEX NAME)



IT **497-19-8**, Sodium carbonate, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(failed reagent in the Suzuki cross-coupling of solid-supported chloropyrimidines with arylboronic acids)
RN 497-19-8 HCAPLUS
CN Carbonic acid disodium salt (8CI, 9CI) (CA INDEX NAME)



●2 Na

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Albericio, F	1990	55	3730	J Org Chem	HCAPLUS
Boojamra, C	1997	62	1240	J Org Chem	HCAPLUS
Breitenbucher, J	2001	3	528	J Comb Chem	HCAPLUS
Breitenbucher, J	1998	39	1295	Tetrahedron Lett	HCAPLUS
Chang, Y	1999	6	361	Chem Biol	HCAPLUS
Ding, S	2002	124	1594	J Am Chem Soc	HCAPLUS
Ding, S	2001	42	8751	Tetrahedron Lett	HCAPLUS
Fantauzzi, P	2000			Abstr Pap Am Chem So	
Franzen, R	2000	78	957	Can J Chem	HCAPLUS
Frenette, R	1994	35	9177	Tetrahedron Lett	HCAPLUS
Gronowitz, S	1986	26	305	Chem Scr	HCAPLUS
Hassan, J	2002	102	1359	Chem Rev	HCAPLUS
Jin, J	2001	3	97	J Comb Chem	HCAPLUS
Johnson, C	1998	54	4097	Tetrahedron	HCAPLUS
Littke, A	1998	37	3387	Angew Chem, Int Ed E	
Littke, A	2000	122	4020	J Am Chem Soc	HCAPLUS
Miyaura, N	1998	6	187	Adv Met Org Chem	HCAPLUS
Parrish, C	2001	66	3820	J Org Chem	HCAPLUS
Pourbaix, C	2001	3	803	Org Lett	HCAPLUS
Wade, J	2001			Abstr Pap Am Chem So	
Wolfe, J	1999	121	9550	J Am Chem Soc	HCAPLUS
Zhang, C	1999	64	3804	J Org Chem	HCAPLUS
Zhang, C	1999	64	3804	J Org Chem	HCAPLUS
Zhang, T	1999	40	5813	Tetrahedron Lett	HCAPLUS

L82 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:625947 HCAPLUS
DN 119:225947
TI Method of synthesis of 1-(2',4',6'-trichlorophenyl)-3-[[2''-chloro-5''-(octadecylsuccinimido)phenyl]amino]-4-(1'''-naphthylazo)pyrazol-5-one by diazo coupling with α-naphthylamine
IN Stepanov, Petr A.; Yurchenko, Galina A.; Khlypenko, Lyubov N.; Stepanova, Galina S.; Zhurin, Robert B.; Dyuzheva, Inna I.
PA Altajskij gni pi khimiko-fotograficheskoj promyshlennosti, USSR
SO U.S.S.R.
From: Izobreteniya 1992, (19), 104.
CODEN: URXXAF
DT Patent
LA Russian
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI SU 1735296	A1	19920523	SU 1990-4821968	19900219 <--
PRAI SU 1990-4821968		19900219 <--		

GI

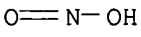
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compound (I) is prepared by reaction of α-naphthylamine with NaNO2 in presence of concentrated HCl at 0 to -2°; the resultant α-naphthyldiazonium chloride is then coupled with pyrazole derivative II in alc. medium in presence of pyridine at 0-35°, in mass ratio α-naphthylamine:II:pyridine = 0.25:1:(1.07-1.60). 2-Propanol is used as solvent. The process is conducted at 15-25°.

IT **7632-00-0**, Sodium nitrite
RL: RCT (Reactant); RACT (Reactant or reagent)
(diazo coupling reagent, for naphthylamine with (trichlorophenyl)[[chloro(octadecylsuccinimido)phenyl]amino]pyrazolone)

RN 7632-00-0 HCAPLUS

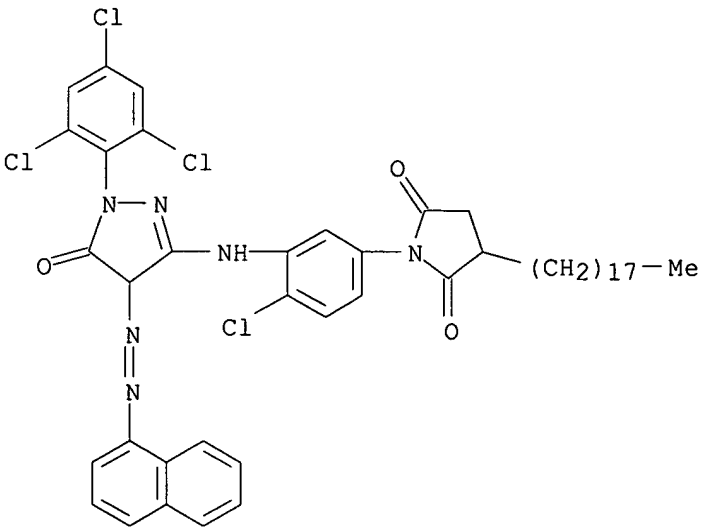
CN Nitrous acid, sodium salt (8CI, 9CI) (CA INDEX NAME)



IT **70207-91-9P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

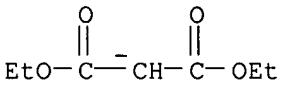
RN 70207-91-9 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[4-chloro-3-[[4,5-dihydro-4-(1-naphthalenylazo)-5-oxo-1-(2,4,6-trichlorophenyl)-1H-pyrazol-3-yl]amino]phenyl]-3-octadecyl- (9CI) (CA INDEX NAME)

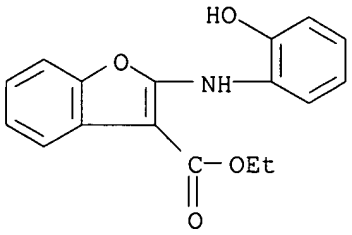


L82 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 1982:423561 HCAPLUS
DN 97:23561

TI Synthesis of benzofuran-2-one derivatives by copper(I)-promoted coupling reactions of o-bromophenol with active methylene compounds
AU Setsune, Junichiro; Matsukawa, Kimihiro; Kitao, Teijiro
CS Dep. Appl. Chem., Univ. Osaka Prefect., Osaka, 591, Japan
SO Tetrahedron Letters (**1982**), 23(6), 663-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 97:23561
AB o-BrC6H4ONa with NaCHRCO2Et (R = CO2Et, COMe, CN) in the presence of CuBr in dioxane at 70 or 80° under N2 for 5 h gave 93% 3-ethoxycarbonylbenzofuran-2-one, 15% 2-hydroxy-3-acetylbenzofuran, and 34% 2-o-hydroxyanilino-3-ethoxycarbonylbenzofuran, resp.
IT **996-82-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction of, with sodium bromophenoxide, benzofuran derivative by cuprous bromide-catalyzed)
RN 996-82-7 HCAPLUS
CN Propanedioic acid, diethyl ester, ion(1-), sodium (9CI) (CA INDEX NAME)



IT **82131-02-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of, by cuprous bromide-catalyzed coupling reaction of bromophenoxide with active methylene compound)
RN 82131-02-0 HCAPLUS
CN 3-Benzofurancarboxylic acid, 2-[(2-hydroxyphenyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



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